Minimal dynamical structure realisations with application to network reconstruction from data

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Abstract— Network reconstruction, i.e., obtaining network structure from data, is a central theme in systems biology, economics, and engineering. Previous work introduced dynamical structure functions as a tool for posing and solving the problem of network reconstruction between measured states. While recovering the network structure between hidden states is not possible since they are not measured, in many situations it is important to estimate the number of hidden states in order to understand the complexity of the network under investigation and help identify potential targets for measurements. Estimating the number of hidden states is also crucial to obtain the simplest state-space model that captures the network structure and is coherent with the measured data. This paper characterises minimal order state-space realisations that are consistent with a given dynamical structure function by exploring properties of dynamical structure functions and developing algorithms to explicitly obtain a minimal reconstruction.

I. Introduction

Networks have received an increasing amount of attention in the last decade. In our "information-rich" world, the questions of network reconstruction and network analysis become crucial for the understanding of complex systems such as biological, social, or economical networks. In particular, the analysis of molecular networks has gained significant interest due to the recent explosion of publicly available high-throughput biological data. In this context, the question of identifying and analysing the network structure at the origin of measured data becomes a key issue.

In some occasions, measured data is given in the form of input-output time-series that describes the effect of inputs on outputs (measured states) of a network. When data is generated by a linear system, a matrix transfer function typically describes the dynamic input-output behaviour and is generally obtained using system identification [6]. If the original state-space model is available or deducible, then the associated network structure can be readily obtained from it. However, a transfer function cannot, in general, recover, or *realise*, the original state-space model since the realisation problem does not typically have a unique solution, i.e. different state-space realisations can generate the same input-output behaviour. Since each of these realisations may suggest entirely different network structures, it is in general impossible to identify network structures from transfer functions alone. Therefore, more information,

beyond input-output data used to identify a transfer function, is needed to prefer one state-space realisation over another as a description of a particular system.

Another difficulty in the network reconstruction problem comes from the fact that the realisation problem becomes ill posed when some of the states are unobservable or "hidden" (this even happens with just one hidden state [8, pp. 78]). As a result, failure to explicitly acknowledge the presence of hidden states and the resulting ambiguity in network structures can lead to a deceptive and erroneous process for network structure discovery. Consequently, determining from measured data the presence or absence of a causal relationship between two variables in a network is a challenging question.

Our previous study [2] introduced the notion of "dynamical structure function" as a representation of an LTI system that encodes structural information at the resolution of the measurements. There we characterised what information, in addition to the transfer function, is necessary and sufficient to uniquely determine the associated dynamical structure function and, consequently, reconstruct the network.

This paper aims to characterise minimal realisations of dynamical structure functions, i.e., minimal order state-space realisations consistent with a given dynamical structure function. In an application, this provides a way to estimate the complexity of the system by determining the minimum number of hidden states in the system. For example, in the context of biology it helps understand the number of unmeasured molecules in a particular pathway: a low number means that most molecules in that pathway have been identified and measured, showing a good understanding of the system; while a large number shows that there are still many unmeasured variables, suggesting that new experiments should be carried out to better characterise that pathway.

The outline of the paper is as follows. Section II reviews the definition of dynamical structure functions and their properties. Section III provides an iterative algorithm to find minimal order realisations for dynamical structure functions based on structure requirements and linear transformations. The main result can be found in Section IV where we introduce a lower complexity heuristic algorithm based on state-space realisations and pole-zero analysis. Conclusions are presented in Section V.

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II. System Model

Consider a nonlinear system $\dot{\bar{x}} = f(\bar{x}, u, w)$, $\bar{y} = h(\bar{x}, w)$ with p measured states $\bar{y}$, hidden states $\bar{z}$ (potentially a large number of them), m inputs u, and noise

w. The system is linearised around an equilibrium point (a point such that $f(\bar{x}^*, 0, 0) = 0$), and it is assumed that inputs and noise do not move the states too far from the equilibrium point so that the linearised system is a valid approximation of the original nonlinear system. The linearised system can be written as $\dot{x} = Ax + Bu$, $y = Cx$, where $x = \bar{x} - \bar{x}^*$ and $y = h(\bar{x}, 0) - h(\bar{x}^*, 0)$. The transfer function associated with this linearised system is given by $G(s) = C(sI - A)^{-1}B$. Typically, we can use standard system identification tools [6] to identify a transfer function $G(s)$ from input-output data.

Like system realisation, network reconstruction also begins with the identification of a transfer function, but it additionally attempts to determine the network structure between measured states without imposing any additional structure on the hidden states. As we have shown in [2], this requires a new representation of linear time-invariant systems. This new representation is obtained as follows: First, we transform $[A, B, C]$ to $\left[A^o, B^o, \left[I_p \ \ 0\right]\right]$ (it is easy to show that this can always be done) and then partition the linear system dynamics as

$$
\begin{bmatrix} \dot{y} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} A_{11}^o & A_{12}^o \\ A_{21}^o & A_{22}^o \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} + \begin{bmatrix} B_1^o \\ B_2^o \end{bmatrix} u \\
y = \begin{bmatrix} I_p & 0 \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix}
\tag{1}
$$

where $x = (y, z) \in \mathbb{R}^{n^o}$, is the full state vector, $y \in \mathbb{R}^p$ is a partial measurement of the state, z are the $n^o - p$ "hidden" states, and $u \in \mathbb{R}^m$ is the control input. In this work we restrict our attention to situations where output measurements constitute partial state information, i.e., $p < n^o$. We consider only systems with full rank transfer functions that do not have entire rows or columns of zeros, since such "disconnected" systems are somewhat pathological and only serve to complicate the exposition without fundamentally altering our conclusions.

Taking the Laplace transforms of the signals in (1) yields

$$
\begin{bmatrix} sY \\ sZ \end{bmatrix} = \begin{bmatrix} A_{11}^o & A_{12}^o \\ A_{21}^o & A_{22}^o \end{bmatrix} \begin{bmatrix} Y \\ Z \end{bmatrix} + \begin{bmatrix} B_1^o \\ B_2^o \end{bmatrix} U
\tag{2}
$$

where Y, Z, and U are the Laplace transforms of y, z, and u, respectively. Solving for Z gives

$$
Z = (sI - A_{22}^o)^{-1} A_{21}^o Y + (sI - A_{22}^o)^{-1} B_2^o U
$$

Substituting this last expression of Z into (2) then yields

$$
sY = W^o Y + V^o U
\tag{3}
$$

where $W^o = A_{11}^o + A_{12}^o (sI - A_{22}^o)^{-1} A_{21}^o$ and $V^o = A_{12}^o (sI - A_{22}^o)^{-1} B_2^o + B_1^o$. Let D^o be a diagonal matrix with the diagonal term of W^o on its diagonal, i.e., $D^o = \text{diag}\{W^o\} = \text{diag}(W_{11}^o, W_{22}^o, ..., W_{pp}^o)$. We thus obtain:

$$
(sI - D^o) Y = (W^o - D^o) Y + V^o U
$$

Note that $W^o - D^o$ is a matrix with zeros on its diagonal. We then have

$$
Y = QY + PU
\tag{4}
$$

where

$$
Q = (sI - D^o)^{-1} (W^o - D^o)
\tag{5}
$$

and

$$
P = (sI - D^o)^{-1} V^o
\tag{6}
$$

Note that Q is zero on the diagonal.

Definition 1: Given the system (1), we define the *dynamical structure function* of the system to be (Q, P), where Q and P are the *internal structure* and *control structure*, respectively, as defined in (5) and (6).

Note that, in general, $Q(s)$ and $P(s)$ carry a lot more information than $G(s)$, which can be seen by the equality $G = (I - Q)^{-1}P$ (see [2] for details). However, $Q(s)$ and $P(s)$ carry less information than the state-space model.

Definition 2: A dynamical structure function, (Q, P), is said to be *consistent* with a particular transfer function, G, if there exists a realisation of G, of some order, and of the form (1), such that (Q, P) are specified by (5) and (6). Likewise, a realisation is consistent with (Q, P) if that realisation gives (Q, P) from (5) and (6).

Definition 3: Consider a system characterised by a transfer function G. The dynamical structure of the system can be *reconstructed*, if there is only one admissible dynamical structure function, (Q, P), that is consistent with G. A realisation of the dynamical structure function is defined as *reconstruction*. Likewise, the Boolean structure of the system can be reconstructed if all admissible dynamical structure functions that are consistent with G have the same Boolean structure.

Given only a transfer function G, [2] shows that dynamical structure reconstruction is not possible. More information is required, i.e., dynamical structure reconstruction is possible from G if and only if in addition $p - 1$ elements in each column of $[Q \ \ P]^T$ are known that uniquely specify the component of (Q, P) in the nullspace of $[G^T \ \ I]$ (see [2] for more details).

Definition 4: We say that a realisation is G minimal if this realisation corresponds to a minimal realisation of G. We say that a realisation is (Q, P) minimal if this realisation has the smallest order and is consistent with (Q, P).

The underlying principle to find a (Q, P) minimal realisation is to search for a realisation with the minimal number of hidden states.

III. Iterative (Q, P) minimal realisation

This section characterises (Q, P) minimal realisations. We start by giving necessary conditions for realisations to be consistent with (Q, P).

Proposition 1: Given a dynamical system (1) and the associated dynamical structure functions (Q, P) with D^o constructed as explained above (see (1)-(6)), the following conditions must hold

$$
\text{diag}\{A_{11}^o\} = \lim_{s \to \infty} D^o(s);
\tag{7}
$$

$$
A_{11}^o - \text{diag}\{A_{11}^o\} = \lim_{s \to \infty} sQ(s);
\tag{8}
$$

$$
B_1^o = \lim_{s \to \infty} sP(s).
\tag{9}
$$

Proof: Eq. (7) is directly obtained from the definition of $\boldsymbol{D}^o(s)$:

$$\lim_{s\to\infty}\boldsymbol{D}^o(s) = \lim_{s\to\infty}\operatorname{diag}\{\boldsymbol{W}^o(s)\}$$
$$= \operatorname{diag}\{\lim_{s\to\infty}\boldsymbol{W}^o(s)\} = \operatorname{diag}\{\boldsymbol{A}_{11}^o\}$$

Since the proofs for eq. (8) and (9) are very similar, we focus on eq. (8) only. Using the fact that for any square matrix $\boldsymbol{M}$, $(\boldsymbol{I}-\boldsymbol{M})^{-1}=\sum_{i=0}^\infty \boldsymbol{M}^i$, we obtain, from the definition of $\boldsymbol{Q}$ given in (5), $\boldsymbol{Q}(s)=\sum_{i=1}^\infty s^{-i}\boldsymbol{D}^{o\ i-1}(\boldsymbol{W}^o-\boldsymbol{D}^o)$ and $\boldsymbol{W}^o = \boldsymbol{A}_{11}^o + \sum_{i=1}^\infty s^{-i}\boldsymbol{A}_{12}^o\boldsymbol{A}_{22}^{o\ i-1}\boldsymbol{A}_{21}^o$. Hence, $\boldsymbol{Q}(s) = (\boldsymbol{A}_{11}^o - \boldsymbol{D}^o(s))s^{-1} + \boldsymbol{r}(s)$, in which $\boldsymbol{r}(s)$ is a matrix polynomial, whose largest degree is -2. Finally, multiplying by s on both sides and taking the limit as s goes to ∞, results in eq. (8). A similar argument can be used to prove eq. (9). ∎

Remark 1: Proposition 1 concludes that all the realisations consistent with $(\boldsymbol{Q},\boldsymbol{P})$ share the same matrices $\boldsymbol{A}_{11}^o$ (minus its diagonal) and $\boldsymbol{B}_1^o$ in eq. (1). Hence, it constraints realisations consistent with $(\boldsymbol{Q},\boldsymbol{P})$.

There exists many realisations consistent with $(\boldsymbol{Q},\boldsymbol{P})$. In the following sections, we focus on finding a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation, i.e., a realisation which is consistent with $(\boldsymbol{Q},\boldsymbol{P})$ and which has minimal order (and hence with the lowest possible complexity). To find a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation, we will proceed in two steps:

1) Get a lower bound on the order of $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisations;
2) Obtain a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation.

A. Lower bound on the order of $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisations

Given $(\boldsymbol{Q},\boldsymbol{P})$, the associated transfer function is given by $\boldsymbol{G}=(\boldsymbol{I}-\boldsymbol{Q})^{-1}\boldsymbol{P}$ (see [2]). Any realisation consistent with $(\boldsymbol{Q},\boldsymbol{P})$ must also be consistent with $\boldsymbol{G}$. Consider a realisation of $\boldsymbol{G}$ given by $\left(\boldsymbol{A},\boldsymbol{B},\boldsymbol{C}=\begin{bmatrix}\boldsymbol{I}_p & 0\end{bmatrix}\right)$ (this form of $\boldsymbol{C}$ can always be obtained with a linear transformation). As a short hand notation, we refer to this realisation as $(\boldsymbol{A},\boldsymbol{B})$. Note that any linear transformation of the form $\left(\boldsymbol{T}^{-1}\boldsymbol{A}\boldsymbol{T},\boldsymbol{T}^{-1}\boldsymbol{B},\begin{bmatrix}\boldsymbol{I}_p & 0\end{bmatrix}\boldsymbol{T}\right)$ with

$$\boldsymbol{T}=\begin{bmatrix}\boldsymbol{I}_p & \boldsymbol{0}_{p\times(n-p)}\\ \boldsymbol{T}_1 & \boldsymbol{T}_2\end{bmatrix}, \tag{10}$$

where n is the dimension of $\boldsymbol{A}$, preserves $\boldsymbol{C}=\begin{bmatrix}\boldsymbol{I}_p & 0\end{bmatrix}$.

The order n of a $\boldsymbol{G}$ minimal realisation is a lower bound on the order of a realisation consistent with $(\boldsymbol{Q},\boldsymbol{P})$. To obtain a tighter lower bound, we can start with realisations of $\boldsymbol{G}$ of order n and iteratively increase the realisation order until we obtain a realisation satisfying the necessary conditions in Proposition 1. Indeed, for a given system order, whenever it is not possible to find a matrix $\boldsymbol{T}_1$ in eq. (10) such that

$$\boldsymbol{A}_{11}+\boldsymbol{A}_{12}\boldsymbol{T}_1-\operatorname{diag}\{\boldsymbol{A}_{11}+\boldsymbol{A}_{12}\boldsymbol{T}_1\}=\lim_{s\to\infty}s\boldsymbol{Q}(s), \tag{11}$$

then according to Proposition 1 this system order is not large enough to obtain a realisation consistent with $(\boldsymbol{Q},\boldsymbol{P})$ and, as a consequence, the order of the realisation must

be increased. This can be seen by applying a linear transformation of the form (10) to the system realisation under consideration, yielding $\left(\boldsymbol{T}^{-1}\boldsymbol{A}\boldsymbol{T},\boldsymbol{T}^{-1}\boldsymbol{B},\begin{bmatrix}\boldsymbol{I}_p & 0\end{bmatrix}\boldsymbol{T}\right)=\left(\boldsymbol{T}^{-1}\boldsymbol{A}\boldsymbol{T},\boldsymbol{T}^{-1}\boldsymbol{B},\begin{bmatrix}\boldsymbol{I}_p & 0\end{bmatrix}\right)$. Partitioning $\boldsymbol{T}^{-1}\boldsymbol{A}\boldsymbol{T}$ as in (1) results in entry $(1,1)$ being $\boldsymbol{A}_{11}+\boldsymbol{A}_{12}\boldsymbol{T}_1$. The result now follows from Proposition 1.

The iterative order increase procedure described above is illustrated in the following example.

Example 1: In this example, the goal is to find a minimal realisation consistent with the following dynamical structure function:

$$[\boldsymbol{Q}\mid\boldsymbol{P}]=\begin{bmatrix}0 & \frac{1}{s+2} & \frac{1}{s+3} & \mid & \frac{1}{s+4}\\ \frac{1}{s+1} & 0 & \frac{1}{s+3} & \mid & \frac{1}{s+4}\\ \frac{1}{s+1} & \frac{1}{s+2} & 0 & \mid & \frac{1}{s+4}\end{bmatrix}.$$

We start with the order of a minimal realisation of $\boldsymbol{G}=(\boldsymbol{I}-\boldsymbol{Q})^{-1}\boldsymbol{P}$, which is four in this case. This corresponds to assuming that there is only one hidden state since $n=4$ and $p=3$. It can be shown that there is no $\boldsymbol{T}_1$ satisfying the requirements of Proposition 1, which means that this order is not large enough. We thus iteratively increase the order of the system until the conditions of Proposition 1 are satisfied. Realising $\boldsymbol{G}$ as a 5th order system (non-minimally), i.e., with two hidden states, again there is no $\boldsymbol{T}_1$ satisfying the requirements of Proposition 1. With a 6th order realisation of $\boldsymbol{G}$ (three hidden states), however, the submatrix $\boldsymbol{A}_{12}$ is full rank showing that there exists a $\boldsymbol{T}_1$ satisfying the conditions of Proposition 1. Hence, we conclude that the order of a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation must be at least $n=6$, implying the existence of at least three hidden states in the system. The next section gives a procedure to verify whether this is a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation or not.

B. $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation

The previous subsection showed how to obtain a lower bound on the order of $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisations. The next step is to obtain an explicit form for a $(\boldsymbol{Q},\boldsymbol{P})$ minimal realisation.

To start, notice that for a given realisation and a linear transformation with $\boldsymbol{T}_1=\boldsymbol{0}$ in eq. (10), the dynamical structure function $(\boldsymbol{Q},\boldsymbol{P})$ is the same for any non-singular $\boldsymbol{T}_2$ [2]. Thus, without loss of generality we can set $\boldsymbol{T}_2=\boldsymbol{I}_n$.

The nominal system $(\boldsymbol{A},\boldsymbol{B})$ after a linear transformation by a $\boldsymbol{T}$ in eq. (10) with $\boldsymbol{T}_2=\boldsymbol{I}_n$ becomes

$$\begin{bmatrix}\boldsymbol{I}_p & \boldsymbol{0}_{p\times(n-p)}\\ -\boldsymbol{T}_1 & \boldsymbol{I}_n\end{bmatrix}\begin{bmatrix}\boldsymbol{A}_{11} & \boldsymbol{A}_{12}\\ \boldsymbol{A}_{21} & \boldsymbol{A}_{22}\end{bmatrix}\begin{bmatrix}\boldsymbol{I}_p & \boldsymbol{0}_{p\times(n-p)}\\ \boldsymbol{T}_1 & \boldsymbol{I}_n\end{bmatrix}$$
$$=\begin{bmatrix}\boldsymbol{A}_{11}+\boldsymbol{A}_{12}\boldsymbol{T}_1 & \boldsymbol{A}_{12}\\ \boldsymbol{A}_{21}-\boldsymbol{T}_1\boldsymbol{A}_{11}-\boldsymbol{T}_1\boldsymbol{A}_{12}\boldsymbol{T}_1+\boldsymbol{A}_{22}\boldsymbol{T}_1 & \boldsymbol{A}_{22}-\boldsymbol{T}_1\boldsymbol{A}_{12}\end{bmatrix}.$$

Note that in general this linear transformation changes the dynamical structure function $(\boldsymbol{Q},\boldsymbol{P})$. The objective is to determine whether it is possible to choose $\boldsymbol{T}_1$ so that the corresponding realisation is compatible with the desired dynamical structure function $(\boldsymbol{Q},\boldsymbol{P})$. We first calculate $\boldsymbol{W}$

as in eq. (3):

$$W = A_{11} + A_{12}T_1 + A_{12}(sI + T_1A_{12} - A_{22})^{-1}$$
$$(-T_1A_{11} + A_{21} - T_1A_{12}T_1 + A_{22}T_1)$$
$$= A_{11} - A_{12}(sI + T_1A_{12} - A_{22})^{-1}(-sT_1 + T_1A_{11} - A_{21})$$
$$= A_{11} + A_{12}[(sI - A_{22})^{-1} - (sI - A_{22})^{-1}T_1(I + A_{12}$$
$$(sI - A_{22})^{-1}T_1)^{-1}A_{12}(sI - A_{22})^{-1}] (T_1(A_{11} - sI) - A_{21})$$

Let $\Omega = A_{12}(sI - A_{22})^{-1}T_1$ and $\bar{W} = A_{12}(sI - A_{22})^{-1}A_{21} + A_{11}$. Notice that $\bar{W}$ is the "W" for the unchanged system, i.e., the system corresponding to $T = I$. We then have

$$W = \bar{W} - \Omega(I + \Omega)^{-1}(\bar{W} - A_{11}) - \Omega(A_{11} - sI)$$
$$+ \Omega(I + \Omega)^{-1}\Omega(A_{11} - sI)$$
$$= sI + (I + \Omega)^{-1}(\bar{W} - sI)$$
$$\Rightarrow sI - W = (I + \Omega)^{-1}(sI - \bar{W}).$$

Hence,

$$I - Q = (sI - D)^{-1}(sI - W) \qquad (12)$$
$$= \left(\text{diag}\{(I + \Omega)^{-1}(sI - \bar{W})\}\right)^{-1} (I + \Omega)^{-1}(sI - \bar{W})$$

In (12), the desired Q is rewritten as a function of T_1 (in the expression of Ω). Given (Q, P) and a realisation of fixed order of $G = (I - Q)^{-1}P$, we can determine whether there exists a nonzero matrix T_1 (in Ω) such that eq. (12) is satisfied. If such a matrix T_1 can be found then there exists a linear transformation T that, when applied to the realisation of fixed order of G results in a realisation consistent with the desired (Q, P).

Based on the theoretical analysis above, the following iterative algorithm can be used:

Algorithm 1: Given a dynamical structure function (Q, P), with corresponding matrix transfer function $G = (I - Q)^{-1}P$, we can find a (Q, P) minimal realisation as follows:

Step 1: Find a minimal realisation (A, B) of G with $C = [I_p \quad 0]$.

Step 2: Determine whether there exists a matrix T_1 such that

$$A_{11} + A_{12}T_1 - \text{diag}\{A_{11} + A_{12}T_1\} = \lim_{s \to \infty} sQ(s). \quad (13)$$

If such a matrix exists go to the next step. Otherwise, increase the order realisation until we obtain a (possibly non-minimal) realisation for G such that a matrix T_1 satisfying the equality (13) can be found.

Step 3: Use eq. (12) to determine whether there exists a linear transformation of the considered realisation which allows one to obtain the desired (Q, P). If yes, use the corresponding transformation matrix to return (A, B) as the (Q, P) minimal realisation and stop. Otherwise, increase the order of the realisation of G until such a linear transformation can be found.

Remark 2: Step 2 serves as a sufficient condition for the (Q, P) minimal realisation while Step 3 provides a necessary condition.

Although this algorithm can find a (Q, P) minimal realisation, it is computationally expensive. The complexity of the last step increases very quickly with the order of the system. The next section provides a lower complexity algorithm.

IV. ALGORITHM TO FIND A (Q, P) MINIMAL REALISATION

From a dynamical structure function (Q, P) we cannot reconstruct (W^o, V^o) since there is no information regarding the diagonal transfer function matrix D^o. This section discusses properties of realisations obtained from transfer function matrices (W, V) consistent with (Q, P). We start with an arbitrarily chosen D, and then use a state-space realisation approach to find a D which minimises the order of a minimal realisation of $[W \quad V] = [(sI-D)Q+D \quad (sI-D)P]$.

Given (Q, P) and a diagonal proper transfer function matrix D, consider a minimal realisation of $[W \quad V] = [(sI - D)Q + D \quad (sI - D)P]$. Partition this realisation as follows [4]:

$$[W \quad V] = [A_{11} \quad B_1] + A_{12}(sI - A_{22})^{-1}[A_{21} \quad B_2] \quad (14)$$

Lemma 1: Given a dynamical structure function (Q, P) and a diagonal proper transfer matrix D, the realisation (A, B) obtained from eq. (14) is consistent with (Q, P) and the pair $(A, [I_p \quad 0])$ is observable.

Proof: The consistency of the realisation with (Q, P) follows from the definition of (Q, P). From the Popov-Belevitch-Hautus (PBH) rank test [8], a matrix pair $(A \in \mathbb{R}^{l \times l}, C)$ is observable iff

$$\text{rank} \begin{bmatrix} sI - A \\ C \end{bmatrix} = l, \qquad (15)$$

for all $s \in \mathbb{C}$. A minimal realisation of $[W \quad V]$ implies that the pair (A_{22}, A_{12}) is observable, i.e.,

$$\text{rank} \begin{bmatrix} sI_{l-p} - A_{22} \\ A_{12} \end{bmatrix} = l - p,$$

Hence

$$\text{rank} \begin{bmatrix} sI - A_{11} & -A_{12} \\ -A_{21} & sI_{l-p} - A_{22} \\ I_p & 0_{p \times (l-p)} \end{bmatrix} = l,$$

which concludes the proof. ∎

Remark 3: Given matrices A and B obtained in eq. (14), the dimension of A is equal to the dimension of a minimal realisation of G iff the pair (A, B) is controllable.

Lemma 2: Suppose W, A_{22} and A are defined in eq. (14), then V and G share the same zeros.

Proof: Since $sI - W$ is the Schur complement of $sI - A_{22}$ in $sI - A$, then

$$\det(sI - W) = \frac{\det(sI - A)}{\det(sI - A_{22})}. \qquad (16)$$

From [9] and fact that $(sI - W)G = V$, then V and G share the same zeros. ∎

Given a dynamical structure function (Q, P), a random choice of a proper diagonal transfer function matrix D is

likely to result in additional zeros in $\boldsymbol{V} = (s\boldsymbol{I} - \boldsymbol{D})\boldsymbol{P}$. From Lemma 2, this will lead to additional zeros in $\boldsymbol{G}$ which are associated to uncontrollable eigenvalues of the considered realisation [1]. At this stage the following question arises: how can we find a proper diagonal transfer function matrix $\boldsymbol{D}$ such that a minimal realisation of $[\boldsymbol{W}\ \boldsymbol{V}]$ is a $(\boldsymbol{Q}, \boldsymbol{P})$ minimal realisation? Note that, since there are many choices for $\boldsymbol{D}$ that minimise the order of minimal realisations of $[\boldsymbol{W}\ \boldsymbol{V}]$, a chosen $\boldsymbol{D}$ may be different from $\boldsymbol{D}^o$.

To answer this question, first notice that for all $\boldsymbol{D}$, $[\boldsymbol{W}\ \boldsymbol{V}]$ can be written as

$$[\boldsymbol{W}\ \boldsymbol{V}] = (s\boldsymbol{I} - \boldsymbol{D})s^{-1}[s\boldsymbol{Q}\ s\boldsymbol{P}] + [\boldsymbol{D}\ \boldsymbol{0}]. \quad (17)$$

Assume that all elements in $[\boldsymbol{Q}\ \boldsymbol{P}]$ only have simple poles. This assumption could be relaxed but we adopt it here for simplicity. In this case, we will show that a minimal order realisation of $[\boldsymbol{W}\ \boldsymbol{V}]$ can always be found with a constant matrix $\boldsymbol{D}$.

Proposition 2: Assume that every element of $[\boldsymbol{Q}\ \boldsymbol{P}]$ only has simple poles. A minimal realisation of $[\boldsymbol{W}\ \boldsymbol{V}]$ given by (17) is achieved with a constant diagonal matrix $\boldsymbol{D}$.

Proof: Assume $\boldsymbol{D}$ has at least one term in the diagonal with the degree of numerator greater than 1, e.g., suppose the ith term in $(s\boldsymbol{I} - \boldsymbol{D})s^{-1} = \frac{(s+a)\epsilon_i(s)}{s\phi_i(s)}$ with $a \in \mathbb{R}$ and $deg(\epsilon_i(s)) = deg(\phi_i(s)) \geq 1$, where $deg(\cdot)$ returns the degree of a polynomial. Hence, the multiplication $(s\boldsymbol{I} - \boldsymbol{D})s^{-1}[s\boldsymbol{Q}\ s\boldsymbol{P}]$ will introduce $deg(\phi_i(s))$ new poles and, due the assumption of simple poles, can at most eliminate $deg(\epsilon_i(s)) = deg(\phi_i(s))$ poles. As a consequence, we can change the ith term to $\frac{s+a}{s}$ without increasing the order of the realisation. ∎

If $\boldsymbol{D}$ is a constant matrix, the term $[\boldsymbol{D}\ \boldsymbol{0}]$ in eq. (17) is also a constant matrix. Therefore, the order of a minimal realisation is only determined by $(s\boldsymbol{I} - \boldsymbol{D})s^{-1}[s\boldsymbol{Q}\ s\boldsymbol{P}] \triangleq \boldsymbol{N}[s\boldsymbol{Q}\ s\boldsymbol{P}]$. Thus, finding the optimal $\boldsymbol{D}$ is equivalent to finding a diagonal proper transfer matrix $\boldsymbol{N}$, with corresponding minimal realisation $(\boldsymbol{A}_2, \boldsymbol{B}_2, \boldsymbol{C}_2, \boldsymbol{D}_2)$, such that it cancels as many poles of $[s\boldsymbol{Q}\ s\boldsymbol{P}]$ as possible. Next, the algorithm is explained step by step.

Step 1: Find a Gilbert's Realisation of the Dynamical Structure Function.
First we find a minimal realisation $(\boldsymbol{A}_1, \boldsymbol{B}_1, \boldsymbol{C}_1, \boldsymbol{D}_1)$ of $[s\boldsymbol{Q}\ s\boldsymbol{P}]$. If $[s\boldsymbol{Q}\ s\boldsymbol{P}]$ has l simple poles, using Gilbert's realisation [5] gives

$$[s\boldsymbol{Q}\ s\boldsymbol{P}] = \sum_{i=1}^{l} \frac{\boldsymbol{K}_i}{s - \lambda_i} + \lim_{s \to \infty}[s\boldsymbol{Q}\ s\boldsymbol{P}], \quad (18)$$

where $\boldsymbol{K}_i = \lim_{s \to \infty}(s - \lambda_i)[s\boldsymbol{Q}\ s\boldsymbol{P}]$ and has rank r_i. For simplicity, we assume that $\boldsymbol{K}_i$ are rank 1 matrices, i.e., $r_i = 1$ for all i. The complex cases for which $r_i \geq 1$ are considered in [11].

Consider a matrix decomposition of $\boldsymbol{K}_i$ in the following form:

$$\boldsymbol{K}_i = \boldsymbol{E}_i\boldsymbol{F}_i, \ \forall i, \quad (19)$$

where $\boldsymbol{E}_i \in \mathbb{R}^l$ and $\boldsymbol{F}_i = (\boldsymbol{E}_i^T \boldsymbol{E}_i)^{-1} \boldsymbol{E}_i^T \boldsymbol{K}_i$. Then $\boldsymbol{A}_1 = \text{diag}\{\lambda_i\} \in \mathbb{R}^{l \times l}$, $\boldsymbol{B}_1 = \begin{bmatrix} \boldsymbol{F}_1^T & \boldsymbol{F}_2^T & \dots & \boldsymbol{F}_l^T \end{bmatrix}^T$, $\boldsymbol{C}_1 = \begin{bmatrix} \boldsymbol{E}_1 & \boldsymbol{E}_2 & \dots & \boldsymbol{E}_l \end{bmatrix}$ and $\boldsymbol{D}_1 = \lim_{s \to \infty}[s\boldsymbol{Q}\ s\boldsymbol{P}]$.

Step 2: Find the Number of Maximal Cancelled Poles.
We define Φ as a largest subset of $\{\boldsymbol{E}_1, \cdots, \boldsymbol{E}_l\}$ such that all the elements in Φ are mutually orthogonal. We also define ϕ as the cardinality of Φ. Computationally, ϕ can be obtained using the algorithm presented in the Appendix. We claim that ϕ is equal to the maximum number of poles we can eliminate (the proof is in the Appendix). Therefore, the minimal order of $[\boldsymbol{W}\ \boldsymbol{V}]$ is

$$l - \phi.$$

As a consequence, the order of the minimal reconstruction is the dimension of $\boldsymbol{A}_{11}$ (constant p) plus the minimal dimension of $\boldsymbol{A}_{22}$ (obtained above): $p + l - \phi$.

Step 3: Construct $\boldsymbol{D}$ to obtain the Minimal Reconstruction.
Once we have Φ, using eq. (21) and $\boldsymbol{D} = s\boldsymbol{I} - s\boldsymbol{N}$, we have that $\boldsymbol{N}(\lambda_i)[j, j] = 0$ implies $\boldsymbol{D}[j, j] = \lambda_i$. Consequently, each element in the set Φ will determine at least one element in $\boldsymbol{D}$, this can be served as the way to construct $\boldsymbol{D}$. We will give an illustrative example below:

Example 2: Consider the dynamical structure function $(\boldsymbol{Q}, \boldsymbol{P})$ given Example 1, i.e.,

$$[\boldsymbol{Q}\ |\ \boldsymbol{P}] = \begin{bmatrix} 0 & \frac{1}{s+2} & \frac{1}{s+3} & | & \frac{1}{s+4} \\ \frac{1}{s+1} & 0 & \frac{1}{s+3} & | & \frac{1}{s+4} \\ \frac{1}{s+1} & \frac{1}{s+2} & 0 & | & \frac{1}{s+4} \end{bmatrix}.$$

The above algorithm steps successively yield the following:
Step 1: A minimal Gilbert realisation of $s[\boldsymbol{Q}, \boldsymbol{P}]$ is

$$\boldsymbol{A}_1 = \text{diag}\{-1, -2, -3, -4\}, \ \boldsymbol{B}_1 = \text{diag}\{2, 2, 2, 4\},$$

$$\boldsymbol{C}_1 = \begin{bmatrix} 0 & -1 & -1.5 & -1 \\ -0.5 & 0 & -1.5 & -1 \\ -0.5 & -1 & 0 & -1 \end{bmatrix}, \ \boldsymbol{D}_1 = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{bmatrix}.$$

Step 2: By definition, $\boldsymbol{E}_i = \boldsymbol{C}_1\boldsymbol{v}_i$, (because in this example $r_i = 1$, $\forall\ i \in \{1, 2, 3, 4\}$, for each eigenvalue of $\boldsymbol{A}_1$, there is only one corresponding eigenvector) where $\boldsymbol{v}_i \in \mathbb{R}^4$ has 1 in its ith position and zero otherwise. Thus,

$$\{\boldsymbol{E}_1, \cdots, \boldsymbol{E}_4\} = \left\{ \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\}.$$

Therefore, ϕ is 1 and the order of a minimal realisation of the given dynamical structure function is $p + l - \phi = 3 + 4 - 1 = 6$, which coincides with the solution in Section III.

Step 3: $\boldsymbol{D}$ can be chosen as $\text{diag}\{a, 1, 1\}$, $\text{diag}\{2, a, 2\}$, $\text{diag}\{3, 3, a\}$, or $\text{diag}\{4, 4, 4\}$ for any $a \in \mathbb{R}$. .

V. CONCLUSIONS

In the context of network reconstruction, once the dynamical structure function has been identified, this work provides results for obtaining a minimal order realisation consistent with the obtained dynamical structure function. This yields a way to estimate the complexity of the system by determining the minimum number of hidden states. For

example, in the context of biology it helps understand the number of unmeasured molecules in a particular pathway.

In particular, the paper explored several approaches to obtain a minimal realisation for a given dynamical structure function. To this aim, properties of the dynamical structure functions were investigated and based on them, necessary and sufficient conditions to test the minimality of a realisation have been given. Iterative and heuristic algorithms were implemented as tools to find such minimal realisations.

VI. Acknowledgement

Appendix

Proof: Proof of the claim in Step 2:
Using results from [1], if a pole of $[sQ \quad sP]$, say λ_i, is cancelled by $N = (sI - D)s^{-1}$, then the realisation of the cascade $(sI - D)s^{-1}[sQ \quad sP]$ loses observability. In this case, it follows that there exists nonzero $w = [w_1^T, w_2^T]^T$ such that

$$\begin{bmatrix} A_1 - \lambda_i I & 0 \\ B_2 C_1 & A_2 - \lambda_i I \\ D_2 C_1 & C_2 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = 0.$$

The first equation shows that w_1 is an eigenvector of A_1 corresponding to λ_i. Since A_1 is diagonal, thus $w_1 = \begin{bmatrix} 0 & \dots & 0 & 1_{i^{th}} & 0 & \dots & 0 \end{bmatrix} \in \mathbb{R}^{1 \times l}$. Therefore, we have

$$\begin{bmatrix} A_2 - \lambda_i I & B_2 \\ C_2 & D_2 \end{bmatrix} \begin{bmatrix} w_2 \\ C_1 v_i \end{bmatrix} = 0.$$

Noticing that $C_1 w_i = E_i$ and that

$$\begin{bmatrix} I & 0 \\ -C_2(A_2 - sI)^{-1} & I \end{bmatrix} \begin{bmatrix} A_2 - sI & B_2 \\ C_2 & D_2 \end{bmatrix} = \begin{bmatrix} A_2 - sI & B_2 \\ 0 & N \end{bmatrix} \tag{20}$$

we therefore obtain

$$N(\lambda_i) E_i = 0. \tag{21}$$

In summary, designing D to cancel any pole λ_i of $[sQ \quad sP]$ is equivalent to imposing that eq. (21) holds. The next question is: given $[sQ \quad sP]$ what is the maximal number of poles that can be cancelled by N, i.e., what is the largest number of poles for which eq. (21) is satisfied. To see this, recall that to cancel a pole λ_i, eq. (21) must be satisfied. Furthermore, $E_i[j]$ being nonzero, for some j, implies that there exists at least one nonzero element in the jth row of E_i. In this case, satisfying eq. (21) imposes that the jth diagonal element of $N(\lambda_i)$ is 0, i.e., the jth diagonal element of D is λ_i. In other words, a nonzero element in E_i corresponds to a fixed value in the corresponding diagonal position in D. Since D is a diagonal matrix with constant values on its diagonal then any orthogonal vectors in $\{E_1, \cdots, E_l\}$ do not intervene in the choice of an element in the diagonal of D. ∎

Algorithm to find ϕ and Φ:
As is presented in [10], an undirected graph is denoted by $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ where $\mathcal{V} = \{\nu_1, \dots, \nu_l\}$ is the set of nodes and $\mathcal{E} \subset \mathcal{V} \times \mathcal{V}$ is the set of edges.

For our purposes, we construct an undirected graph $\mathcal{G}_a$ using the following rules:

- A node is associated with each vector in the set $\{E_1, \cdots, E_l\}$. There are thus l nodes in the considered graph.
- An undirected edge (i, j) is drawn between node i and node j if the equality $E_i^T E_j = 0$ is satisfied.

It is easy to see that the maximum cardinality of the set Φ corresponds to the maximum number of nodes in a complete subgraph K_n of the graph $\mathcal{G}_a$. Methods for finding a largest complete subgraph in an undirected graph are well-developed in computer science and some corresponding MATLAB code can be downloaded from [12]. Therefore, we can use these methods to obtain a largest complete subgraph and consequently compute the corresponding set Φ.

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